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**INSTABILITY MECHANISMS OF THERMALLY-DRIVEN INTERFACIAL  
FLOWS IN LIQUID-ENCAPSULATED CRYSTAL GROWTH**

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## SUMMARY OF YEAR-1 ACHIEVEMENTS

During the past year, a great deal of effort was focused on the enhancement and refinement of the computational tools developed as part of our previous NASA grant. In particular, the interface mollification algorithm developed earlier was extended to incorporate the effects of surface-rheological properties in order to allow the study of thermocapillary flows in the presence of surface contamination. These tools will be used in the computational component of the proposed research in the remaining years of this grant. A detailed description of the progress made in this area is provided elsewhere [1, 2]. Briefly, the method developed allows for the convection and diffusion of bulk-insoluble surfactants on a moving and deforming interface. The novelty of the method is its grid independence: there is no need for front tracking, surface reconstruction, body-fitted grid generation, or metric evaluations; these are all very expensive computational tasks in three dimensions. For small local radii of curvature there is a need for local grid adaption so that the smearing thickness remains a small fraction of the radius of curvature. A special Neumann boundary condition was devised and applied so that the calculated surfactant concentration has no variations normal to the interface, and it is hence truly a surface-defined quantity. The discretized governing equations are solved subsequently using a time-split integration scheme which updates the concentration and the shape successively. Results demonstrate excellent agreement between the computed and exact solutions.

In addition to the development of the required computational tools, recent efforts have been focused on the computation of the base flow structure in a differentially-heated rectangular cavity with one free surface. As a means of rapidly generating insight into the nature of these problems, a domain-mapping method has been used to study the generation of vorticity and the resulting motions and surface deformations for both single and double fluid layers in finite aspect-ratio cavities. A vorticity-streamfunction formulation is used for the two-dimensional problems investigated initially. The surface pressure is calculated from the restriction of the Navier-Stokes onto the interface. The specification of stress and kinematic conditions closes the formulation. Several investigators have studied the contact line problem using finite element methods, *while neglecting capillary effects around the contact line* [3, 4].

The immediate goal of these simulations is to shed light on the behavior of an originally pinned interface both in the absence and presence of gravity. In all of these computations, the contact lines have been taken to be initially pinned at knife edges on the solid boundary while allowing the fluid-fluid interface to deform. This steady base flow is then allowed to 'jump' the knife edge. The post-jump evolution of the interface and its parametric dependencies are then investigated. The parameters considered are the Reynolds, Marangoni, capillary, Froude, and Biot numbers, as well as the aspect ratio.

In parallel with the parametric studies for the pinned-interface problem, work has begun on understanding the role of the contact-line condition on the time-dependent

behavior of thermocapillary convection in single and double layer fluid structures in the cavity configuration. Using the steady flow patterns computed earlier (based on the pinned contact-line condition) as initial conditions, we allow the contact lines to move on the solid boundaries using a slip model, and compute the resulting time-dependent flows in order to examine the stability of the computed base flows to contact line movement.

The existence of contact lines in these systems introduces the possibility of a spectrum of instabilities ranging from catastrophic [10], to merely undesirable (Hocking [8], and Davis [7]). The tendency of the contact line to jump the knife edge, and travel up the side walls, striving to achieve minimum surface potential energy, has been modeled by Concus and Finn [5, 6], and discussed by Myshkis et al. [9]. Such tendencies were likely responsible for the failure of the flight experiment of Koster [10], wherein one layer of the three-layer side-heated fluid system was completely engulfed by another. Though not initially catastrophic, the dynamic instabilities of the contact line—investigated by Hocking [8] for a spreading fluid ridge, and by Davis [7] for a fluid rivulet—may indeed grow and bifurcate into finite-amplitude disturbances with the ability to unpin interfaces and lead to catastrophic instabilities. At the very least, these instabilities will give rise to undesirable dopant striations at the interface of the grown crystals. Hence, realistic contact line conditions must be used to account for interface deformations in modeling crystal growth.

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## PRESENTATIONS AND PUBLICATIONS

- **Presentations :**

1. Haj-Hariri, H., and Borhan, A., "Instability mechanisms of thermally-driven interfacial flows in liquid-encapsulated crystal growth," third NASA Fluid Physics Conference, Cleveland, OH, June 1996.

- **Publications :**

1. Haj-Hariri, H. and Borhan, A., "A computational model for surfactant transport on deformable two-phase boundaries based on interface mollification," In *Boundary Elements XVIII*, edited by C. A. Brebbia, J. B. Martins, M. H. Aliabadi, and N. Haie (Computational Mechanics Publications, Southampton, 1996), 541–550.
2. Haj-Hariri, H., Shi, Q., and Borhan, A., "Thermocapillary motion of deformable drops at finite Reynolds and Marangoni numbers," *Phys. Fluids*, 9:845–855, 1997.
3. Haj-Hariri, H. and Homsy, G.M., "Three-dimensional instability of viscoelastic elliptic vortices," *J. Fluid Mech.*, in review.

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